On adaptability and "intermediate phase" in randomly connected networks

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We present a simple model that enables us to analytically characterize a floppy to rigid transition and an associated self-adaptive intermediate phase in a random bond network. In this intermediate phase, the network adapts itself to lower the stress due to constraints. Our simulations verify this picture. We use these insights to identify applications of these ideas in computational problems such as vertex cover and K-SAT.

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The concepts of rigidity and a rigidity transition [1, 2] have been successfully applied to the study of network glasses. The bonds in a network are considered as constraints such that at low connectivity there are more degrees of freedom than constraints, so that the network is flexible, or floppy. At high connectivity, there are more constraints than degrees of freedom, and the network is said to be rigid and stressed. The rigidity transition lies in between and Thorpe *et al.* [3] have recently suggested the idea of *adaptability* of a network to avoid stress, which has led to the discovery of an *intermediate phase*, between the usual floppy and rigid ones. The existence of this phase has been confirmed by numerical studies [3], analysis of finite size clusters [4] and by experiments [5]. What has been lacking is an appropriate model of the intermediate phase that allows for analytical calculations and provides insight. Furthermore, the ingredients at the origin of the intermediate phase are quite generic: adaptability of the underlying network undergoing a transition, so as to avoid stress. This suggests that such intermediate phases may be relevant in many different fields. For instance, links between rigidity theory and computational phase transitions have already been suggested [6], but not examined further than an analogy. The insight gained from the minimal model we discuss here will demonstrate how an intermediate phase can arise in computational problems such as the vertex cover problem [7] or K-SAT [8].

We will first present and solve a simple random bond model for the rigidity transition. We then introduce the possibility of adaptation of the network. Through mean-field calculations, we demonstrate the presence of an intermediate phase and study its properties. The calculations are quantitatively confirmed by Monte Carlo simulations. We then outline how the results could be extended to computational phase transitions.

Very few non-trivial exactly solvable models are available for the standard rigidity transition. To our knowledge, the randomly bonded models, equivalent to Bethe-like lattices [9], are the only ones available. The first idea of this paper is therefore to introduce *adaptability* in the randomly bonded models to obtain a description of the complete phase diagram, including the intermediate phase. We consider a simple model for the rigidity transition. Our network consists of N atoms, $N_3 = Nx_3$ of which are 3-fold coordinated, and $N_1 = Nx_1$ are 1-fold coordinated; we consider bond stretching as well as bond bending constraints. Atoms are bonded randomly, disregarding space: this leads locally to a tree-like network, which allows for analytical calculations [9]; an example with $N = 16$ atoms is given Fig. 1. Our aim is not to accurately describe network glasses, rather to seek a simplified description of the salient features. We invoke the following constraint counting argument: each atom has a priori 3 degrees of freedom (the network is embedded in 3-dimensional space), each 1-atom brings 1/2 constraint (1 bond stretching shared with its neighbor and no bond bending), and each 3-atom brings 9/2 constraints (3/2 bond stretching and 3 bond bending). If no constraint is redundant, the number of unconstrained degrees of freedom (or floppy modes) is given by the Maxwell estimate [1, 2]

$$N_{flop} = 3N - \frac{Nx_1}{2} - \frac{9Nx_3}{2} \ . \qquad (1)$$

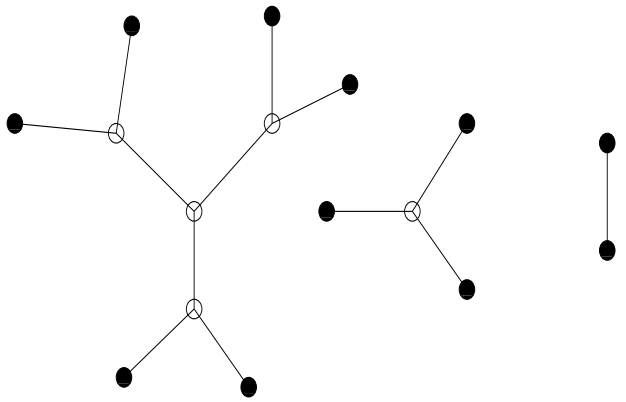

FIG. 1: Example of a network with $N_1 = 11$, $N_3 = 5$, so that $x_3 = 0.3125$. It has $N_{11} = 1$, $N_{13} = 9$, $N_{33} = 3$, $N_3^{(0)} = 1$, $N_3^{(1)} = 3$, $N_3^{(2)} = 0$, $N_3^{(3)} = 1$ (see text). The two subgraphs on the right are rigid; the one on the left has three internal degrees of freedom: the rotations around the $3-3$ bonds. There is no stress in the network.

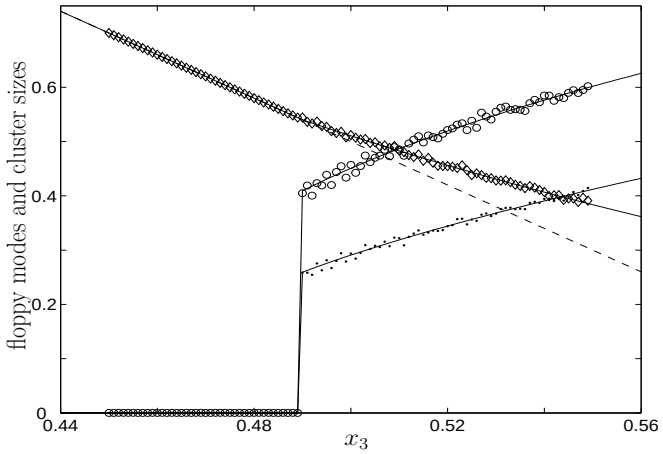

FIG. 2: Comparison of analytical calculations (solid lines) with numerics (symbols). The diamonds represent the number of floppy modes per atom; the circles (dots) the fraction of the network in the percolating rigid (stressed) cluster. The dashed line is the constraint counting estimate for the number of floppy modes. The numerics are performed on networks of 4×10^4 atoms.

This yields the estimate for the transition point $x_3^* \simeq 0.625$, for which the mean number of constraints per atom equals 3, the number of degrees of freedom [10]. The calculation can be carried out exactly using a method developed in [11] or by adapting the cavity formalism originally devised for spin glasses [12]. The cavity method has been used recently [13] to study a computational phase transition: its use is thus the first formal link, beyond a simple analogy, between rigidity theory and the field of computational phase transitions. These calculations confirm the presence of a rigidity transition, first order in this case, at a concentration of 3-atoms (i.e. atoms with three bonds) $x_3^* = 0.490$; see Fig. 2. At the rigidity transition, a macroscopic rigid cluster appears. In the rigid phase, some constraints cannot be fulfilled, and stress is present.

As stress costs energy, it is natural to assume that the network will try to adapt itself to avoid it. To make this idea more precise, let us define a stress energy for a given configuration of the network, equal to the number of redundant constraints, that is constraints that cannot be fulfilled. This energy is of course zero in the floppy phase where all constraints can be accommodated, and non-zero in the rigid phase, as shown on Fig. 2. Constraint counting gives

$$N_{flop} = 3N - \frac{1}{2}N_1 - \frac{9}{2}N_3 + N_{red} \ , \tag{2}$$

where N_{flop} is the number of floppy modes in the network, N_{red} is the number of redundant constraints, $3N$ is the a priori number of degrees of freedom, and $(N_1+9N_3)/2$ is the total number of constraints. Thus, for a fixed concentration of 3-atoms, counting N_{flop} amounts to the same as counting N_{red}. Consequently, in the following, we will use indifferently

$$H = N_{flop} \text{ or } H = N_{red} \ . \tag{3}$$

We assume in addition that the network is adaptive: i.e. while N_1 and N_3 are fixed, some bonds can be rewired to decrease the energy (3), thus moving the network away from the randomly bonded case. The standard rigidity transition described above thus corresponds to the infinite temperature case. At finite temperature, new phenomena arise (below).

To realize the calculations, it is crucial to devise a means to measure the degree of organization or randomness of the network. At the crudest level, this is provided by the number of bonds between two 1-atoms, one 1-atom and one 3-atom, and two 3-atoms, respectively termed N_{11}, N_{13}, N_{33}, see Fig. 1. In the randomly bonded case, a simple calculation shows

$$N_{11} = \frac{N}{2}\frac{x_1^2}{x_1+3x_3} = N_{11}^* \ , \tag{4}$$

$$N_{13} = \frac{N}{2}\frac{6x_1x_3}{x_1+3x_3} = N_{13}^* \ , \tag{5}$$

$$N_{33} = \frac{N}{2}\frac{9x_3^2}{x_1+3x_3} = N_{33}^* \ . \tag{6}$$

At finite temperature, N_{ij} can now deviate from its random value N_{ij}^*, with the constraints $2N_{11} + N_{13} = N_1$ and $2N_{33} + N_{13} = 3N_3$. The level of organization of the network, at this crude one bond level, is thus determined by a single parameter, which we take to be $a = N_{11}/N_{11}^*$. Fixing a fixes all N_{ij}; $a = 1$ corresponds to the random bonding case, and $a \neq 1$ denotes an adaptation of the network. Assuming that there are no correlations in the network beyond the one bond level, the Chubinsky [11] or the cavity methods allow exact calculations of the energy H as a function of x_3 and a. It turns out that the lower a, the higher is the rigidity threshold for x_3. This is intuitive: decreasing the number of dimers of two 1-atoms at fixed x_3 decreases the mean connectivity of the main network, which is then less likely to be rigid. At fixed a, knowing the N_{ij}, it is a simple combinatorial problem to compute the configurational entropy of the network; $S(x_3, a) = Ns(x_3, a) = \ln \Omega$, with

$$\Omega(N_{11}, N_{13}, N_{33}) = \frac{N_1!\ (3N_3)!}{2^{N_{11}}2^{N_{33}}\ N_{11}!\ N_{13}!\ N_{33}!}. \tag{7}$$

The conclusion of the calculation now only amounts to minimizing with respect to the parameter a the free energy $H(x_3, a) - TS(x_3, a)$, at given T and x_3. This step is sketched in Fig. 3. What occurs is again intuitively clear: for $x_3 < x_3^*$, the random network is unstressed, thus entropic and energetic contributions are optimized for $a = 1$, and the energy is zero. For $x_3 > x_3^*$, random bonding has a non-zero energy; however, for small

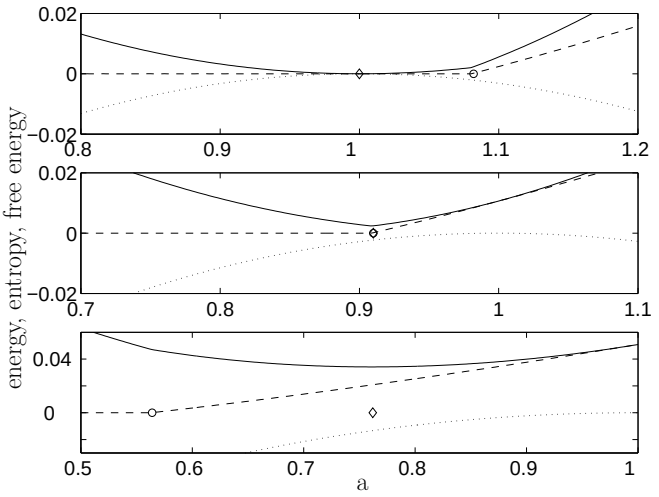

FIG. 3: Energy (dashed line), entropy (dotted line) and free energy (solid line) as a function of the parameter a for different x_3; from top to bottom, $x_3 = 0.48$ (floppy phase), $x_3 = 0.5$ (intermediate phase), $x_3 = 0.53$ (rigid phase). The circle indicates the rigidity transition varying a at fixed x_3; the diamond indicates the free energy minimum; both coincide in the intermediate phase.

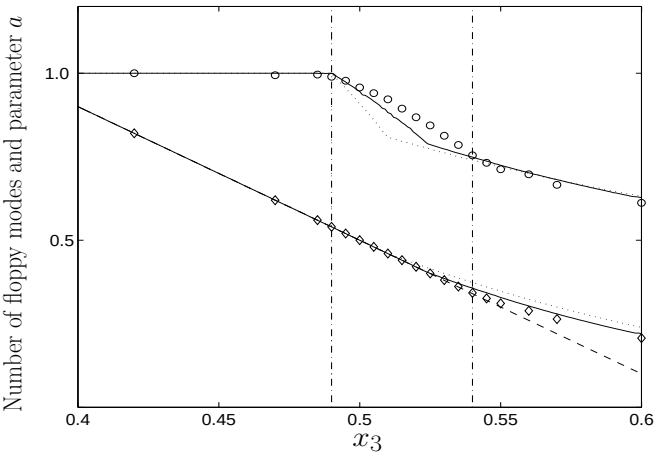

FIG. 4: Comparison between MC simulations (circles for the a parameter, diamonds for the number of floppy modes per atom) and analytical results (dotted lines correspond to the one bond correlation level and solid lines to the two bond correlation level). The two dot-dashed vertical lines indicate the location of the two phase transitions. The dashed line indicates the Maxwell estimate for the number of floppy modes, see eq. (1). MC simulations involve 5000 or 20000 atoms, for 10^6 MC steps.

enough x_3, decreasing a to avoid stress energy costs little entropy, and is favorable. This is the intermediate phase. Throughout this phase, the system adapts itself to stay exactly on the verge of stress, so that the entropic cost is minimal and there is no stress. For x_3 large enough, decreasing a further to avoid stress costs too much entropy, and the appearance of some stress is favored. This happens at a second transition $x_3 = x_3^{**}$. The results are summarized in Fig. 4. To test this proposed scenario, we performed Monte Carlo simulations of the system as follows: at each step, we pick a pair of bonds and rewire them, accepting the move according to the Metropolis algorithm with energy (3), and temperature chosen to be $T = 5$. Choosing another temperature does not induce any qualitative change; only the width of the intermediate phase is affected: the lower the temperature, the wider the intermediate phase. In the limit of a non-adaptive network $T \to \infty$, the intermediate phase disappears. The network is analyzed, when needed, using the pebble game algorithm [14], which gives access to the number of floppy modes, and thus the energy (3), and provides the decomposition of the network into rigid and stressed clusters. We performed simulations on $N = 5000$ and $N = 20000$ systems, for 10^6 Monte Carlo steps. Longer test runs did not show any significant differences. Results for the parameter a and the number of floppy modes, Fig. 4, show a qualitative agreement with the simple calculation above: a floppy phase with $a = 1$ at low x_3, a stressed phase at high x_3 and an intermediate unstressed but self-adapted $a \neq 1$ phase.

The agreement is quantitatively not very good: the assumption of retaining only one bond correlations most likely breaks down. The above calculation can indeed be refined to take into account longer range correlations. The first steps in this direction consist in counting not only the bonds as above, but also the paths along two bonds which are of four types: from 1 to 3 to 1, from 1 to 3 to 3, from 3 to 3 to 1, and from 3 to 3 to 3. This is equivalent to counting $N_3^{(0)}, N_3^{(1)}, N_3^{(2)}, N_3^{(3)}$, the number of 3-atoms that are linked respectively with zero, 1, 2 and 3 other 3-atoms. Since the two equations

$$3N_3^{(0)} + 2N_3^{(1)} + N_3^{(2)} + 2N_{11} = N_1 \quad (8)$$

$$N_3^{(0)} + N_3^{(1)} + N_3^{(2)} + N_3^{(3)} = N_3 \quad (9)$$

must be satisfied, describing the network at the level of two bond correlations requires the introduction of two new parameters, defined as follows:

$$\alpha_0 = \frac{N_3^{(0)}}{N_3^{(0)*}} \quad (10)$$

$$\alpha_1 = \frac{N_3^{(1)}}{N_3^{(1)*}} , \quad (11)$$

where $N_3^{(i)*}$ is the number $N_3^{(i)}$ expected without two bond correlations. Thus, any $\alpha_i \neq 1$ shows the presence of two bond correlations. Using the cavity method, one can calculate the energy $H(x_3, a, \alpha_0, \alpha_1)$. As above with the parameter a, it turns out that the lower α_0 and α_1 are, the less stress-prone is the network. Evaluating the entropy $S(x_3, a, \alpha_0, \alpha_1)$ is still a simple combinatorial problem. The results are plotted in Fig. 4, and are

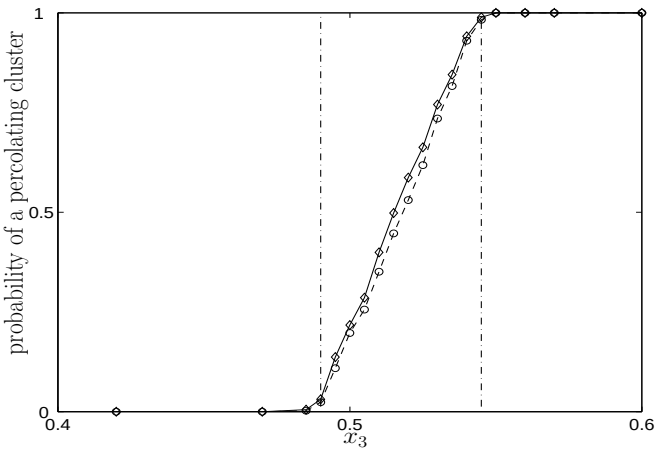

FIG. 5: Diamonds (circles): probability that a rigid (stressed) cluster percolates the entire sample, as a function of x_3. The runs were made with $N = 5000$ or $N = 20000$ atoms, for 10^6 MC steps. Solid and dashed lines are guides for the eyes; dot-dashed lines indicate the location of the two phase transitions.

much closer to the numerical results. Due to the simplicity of the model, we were able to make the calculations up to three bonds correlations; they confirm the trend toward the numerical results, but do not completely coincide with them in the intermediate phase. This leads to the important conclusion that medium or long range correlations are important in the network, especially in the intermediate phase [4].

Monte Carlo simulations also provide the opportunity to examine the different phases in greater detail. The most important question concerns the presence or absence of percolating rigid or stressed clusters. In the floppy phase, there is no percolating rigid or stressed cluster, whereas in the stressed phase rigidity and stress always percolate. The interesting case is the intermediate phase: our simulations show that the probability to find a rigid or stressed percolating cluster varies smoothly from 0 to 1, see Fig. 5. The probability to find a stressed cluster is always slightly lower than the probability to find a rigid one. Thus, while in the intermediate phase the system lies right on the boundary between rigid and floppy, the probability to be on one side or another of the boundary goes from 0 to 1. Although strictly speaking the model gives access only to Monte Carlo sampling of the phase space, we can attempt to infer a dynamical picture of the intermediate phase, namely a percolating rigid cluster disconnecting and reconnecting elsewhere through local connections.

From the detailed analysis above, the ingredients leading to the intermediate phase appear to be clear: an underlying first order phase transition, and the possibility of adaptation of the network, giving rise to an entropy competing with the energy associated with the underlying transition. One thus expects the same phenomena for a variety of computational phase transitions. Consider the vertex cover problem as an example. The problem is as follows: given a network of size N, is it possible to find a subset of vertices of size xN, such that all edges are adjacent to this subset? Such a subset is called a vertex cover. If the network structure is random and fixed, this is always possible at low connectivity, and becomes impossible at high enough connectivity [7], through a phase transition. If one defines the energy of a configuration as the number of edges not adjacent to the subset chosen, and allows for a reorganization of the network, an intermediate phase with a finite probability of finding a vertex cover is likely to appear. This should apply also to satisfiability problems of the K-SAT type [8]. More generally, as most networks found in physics, social science or biology, are adaptive, the intermediate phase described in this work is likely to be encountered in a wide variety of situations. Future work will elaborate the thermodynamic and dynamical signatures of the intermediate phase, including expectations of filamentary geometry and glassiness.

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